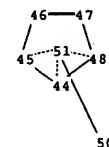
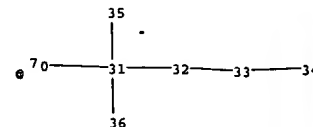
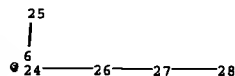
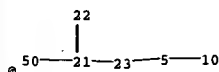
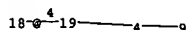
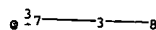
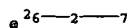
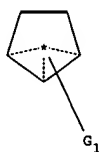
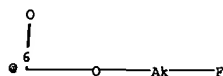
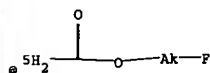
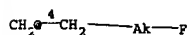
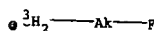
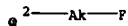
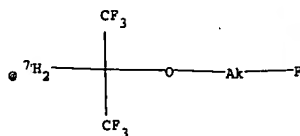


9/24/01



chain nodes :

1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 22 23 24 25 26 27 28 30 31
32 33 34 35 36 50

ring nodes :

44 45 46 47 48

chain bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

ring bonds :

44-45 44-48 45-46 46-47 47-48

exact/norm bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 26-27 27-28 31-32 32-33 33-34 46-47
47-48

exact bonds :

18-19 20-21 21-22 21-23 24-25 24-26 30-31 31-35 31-36 44-45 44-48 45-46

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS 28:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
35:CLASS 36:CLASS 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 50:CLASS 51:CLASS

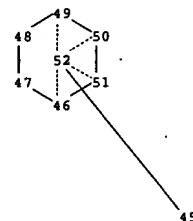
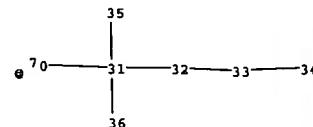
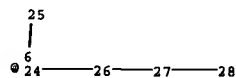
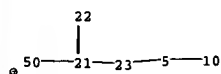
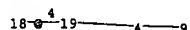
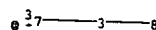
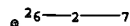
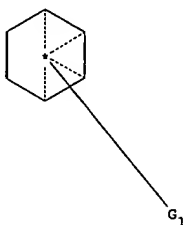
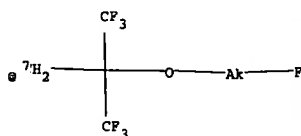
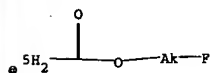
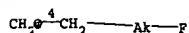
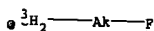
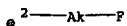
Element Count :

Node 1: Limited
C,C1-6Node 2: Limited
C,C1-6Node 3: Limited
C,C1-6

. Node, 4: Limited
C,C1-6

Node 5: Limited
C,C1-6

Node 27: Limited
C,C1-6



chain nodes :

1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 22 23 24 25 26 27 28 30 31
32 33 34 35 36 45

ring nodes :

46 47 48 49 50 51

chain bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

ring bonds :

46-47 46-51 47-48 48-49 49-50 50-51

exact/norm bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 26-27 27-28 31-32 32-33 33-34 47-48
48-49

exact bonds :

18-19 20-21 21-22 21-23 24-25 24-26 30-31 31-35 31-36 46-47 46-51 49-50 50-51

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS 28:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS
35:CLASS 36:CLASS 45:CLASS 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:CLASS
52:CLASS

Element Count :

Node 1: Limited
C,C1-6Node 2: Limited
C,C1-6Node 3: Limited
C,C1-6

68

783

6531260

65 200 1041769 = 824224

6468712

4503684

Node 4: Limited
C,C1-6

Node 5: Limited
C,C1-6

Node 27: Limited
C,C1-6

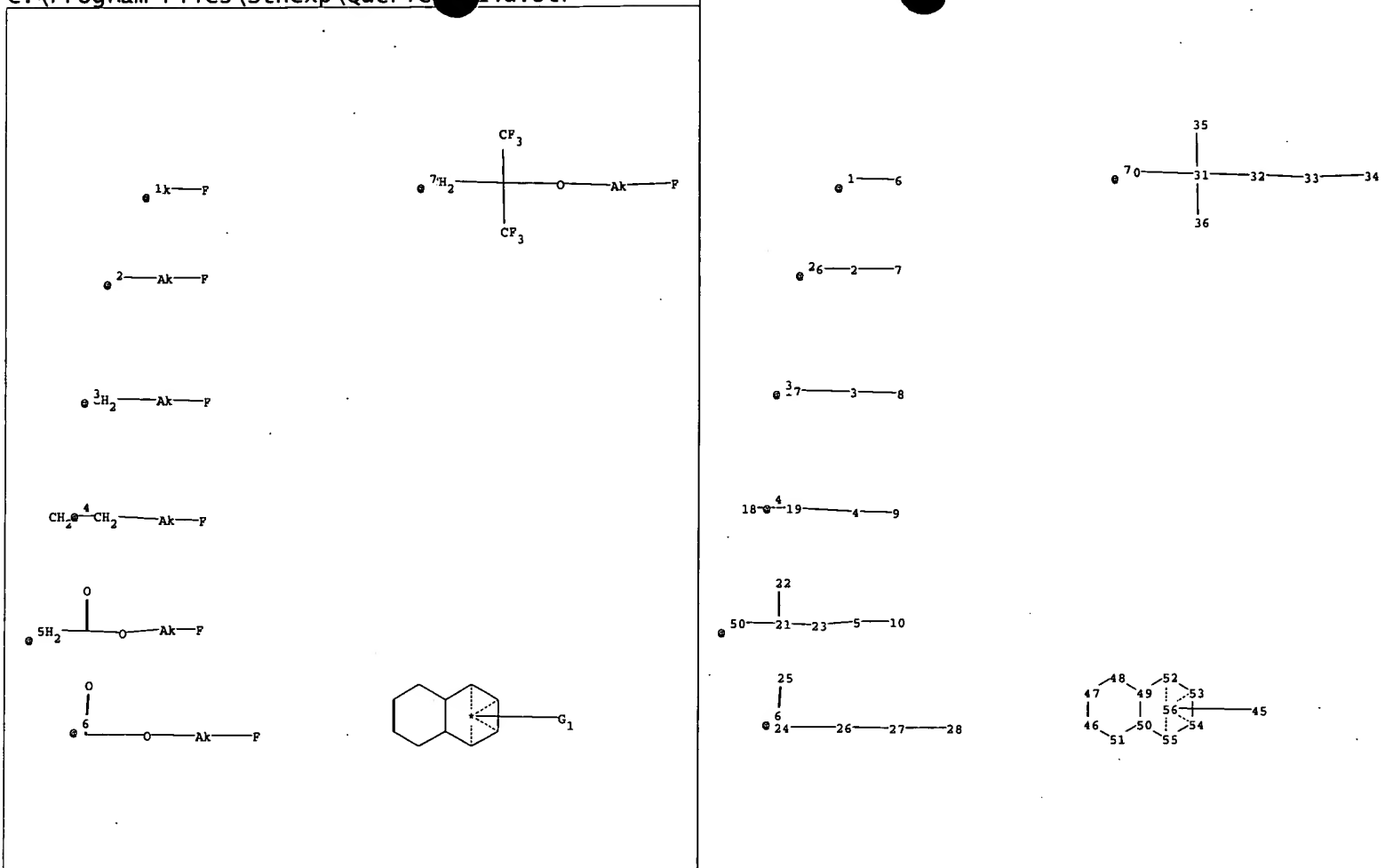
783 446.99.

6579 458 220 ?

824224

65 31260

646 8712



chain nodes :

1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 22 23 24 25 26 27 28 30 31
32 33 34 35 36 45

ring nodes :

46 47 48 49 50 51 52 53 54 55

chain bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

ring bonds :

46-47 46-51 47-48 48-49 49-50 49-52 50-51 50-55 52-53 53-54 54-55

exact/norm bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 21-22 21-23 24-25 24-26 26-27 27-28
31-32 32-33 33-34

exact bonds :

18-19 20-21 30-31 31-35 31-36 46-47 46-51 47-48 48-49 49-50 49-52 50-51 50-55
52-53 53-54 54-55

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 16:Atom
17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS
26:CLASS 27:CLASS 28:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS
36:CLASS 45:CLASS 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom
54:Atom 55:Atom 56:CLASS

Element Count :

Node 1: Limited
C,C1-6

Node 2: Limited
C,C1-6

Node 3: Limited

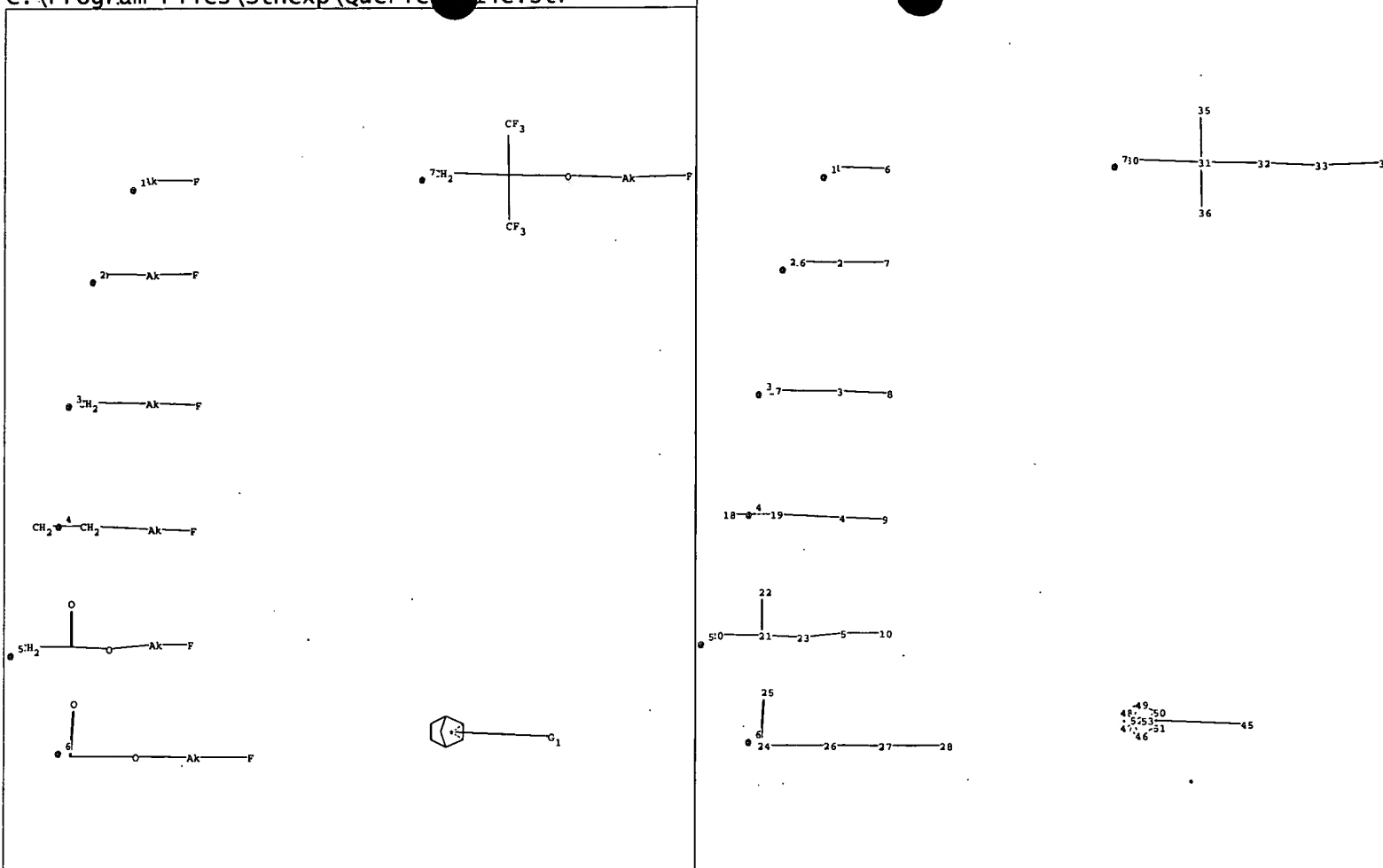
824 224
= 6531240

C,C1-6

Node 4: Limited
C,C1-6

Node 5: Limited
C,C1-6

Node 27: Limited
C,C1-6



chain nodes :

[illegible]

ring nodes :

46 47 48 49 50 51 52

chain bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

ring bonds :

46-47 46-51 46-52 47-48 48-49 49-50 49-52 50-51

exact/norm bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 21-22 21-23 24-25 24-26 26-27 27-28
31-32 32-33 33-34

exact bonds :

18-19 20-21 30-31 31-35 31-36 46-47 46-51 46-52 47-48 48-49 49-50 49-52 50-51

G1: [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 16:Atom
17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
27:Atom 28:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom

```

Element Count :

Node 1: Limited
C,C1-6

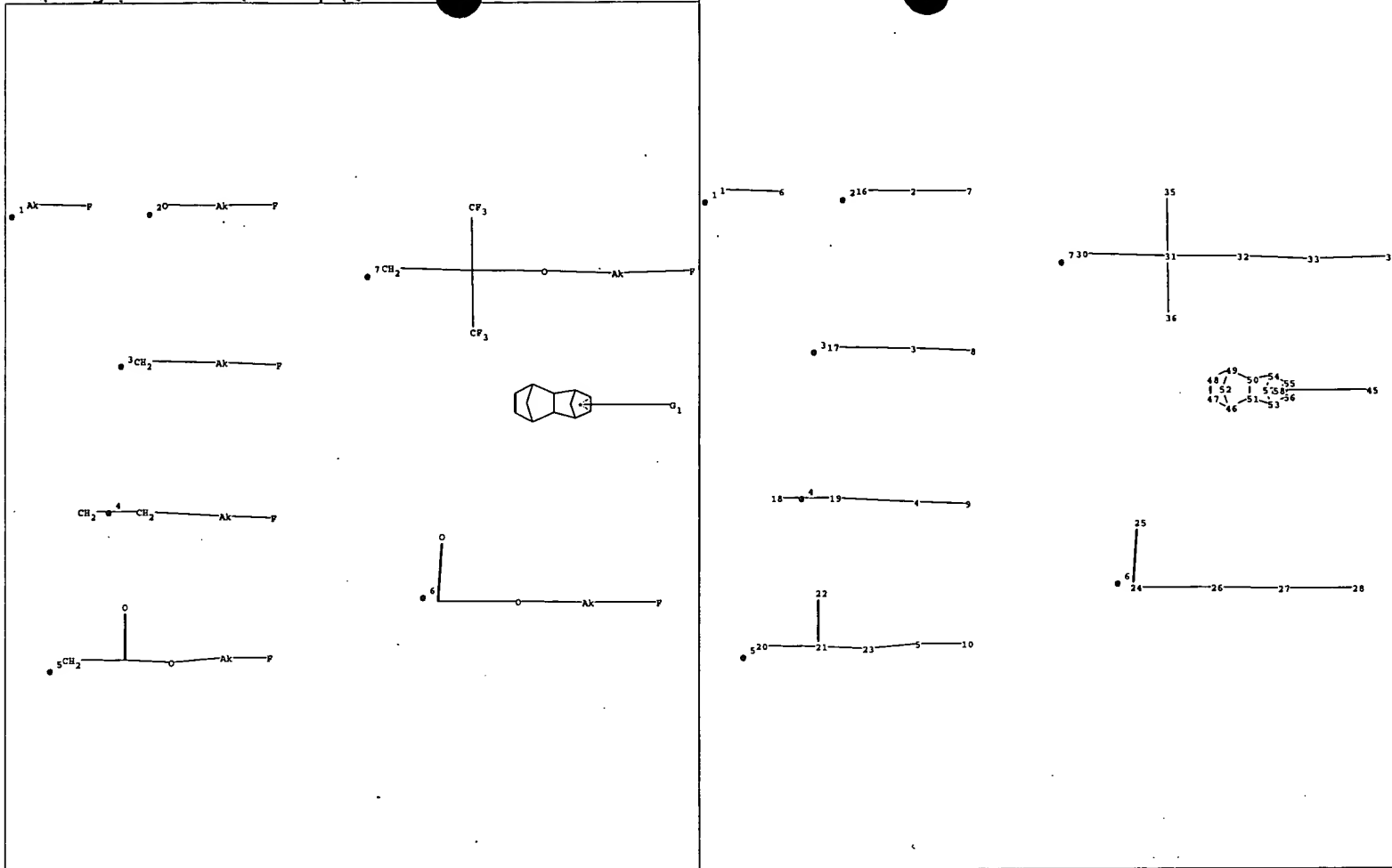
Node 2: Limited
C,C1-6

Node 3: Limited
C,C1-6

Node 4: Limited
C,C1-6

Node 5: Limited
C,C1-6

Node 27: Limited
C,C1-6



chain nodes :

1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 22 23 24 25 26 27 28 30 31
32 33 34 35 36 45

ring nodes :

46 47 48 49 50 51 52 53 54 55 56 57

chain bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

ring bonds :

[illegible]

exact/norm bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 21-22 21-23 24-25 24-26 26-27 27-28
31-32 32-33 33-34

exact bonds :

18-19	20-21	30-31	31-35	31-36	46-47	46-51	46-52	47-48	48-49	49-50	49-52	50-54
50-51	51-53	53-57	53-56	54-57	54-55	55-56						

G1: [*1], [*2], [*3], [*4], [*5], [*6], [*7]

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 16:Atom
17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
27:Atom 28:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom
56:Atom 57:Atom 58:CLASS

```

Element Count :

Node 1: Limited
C.C1-6

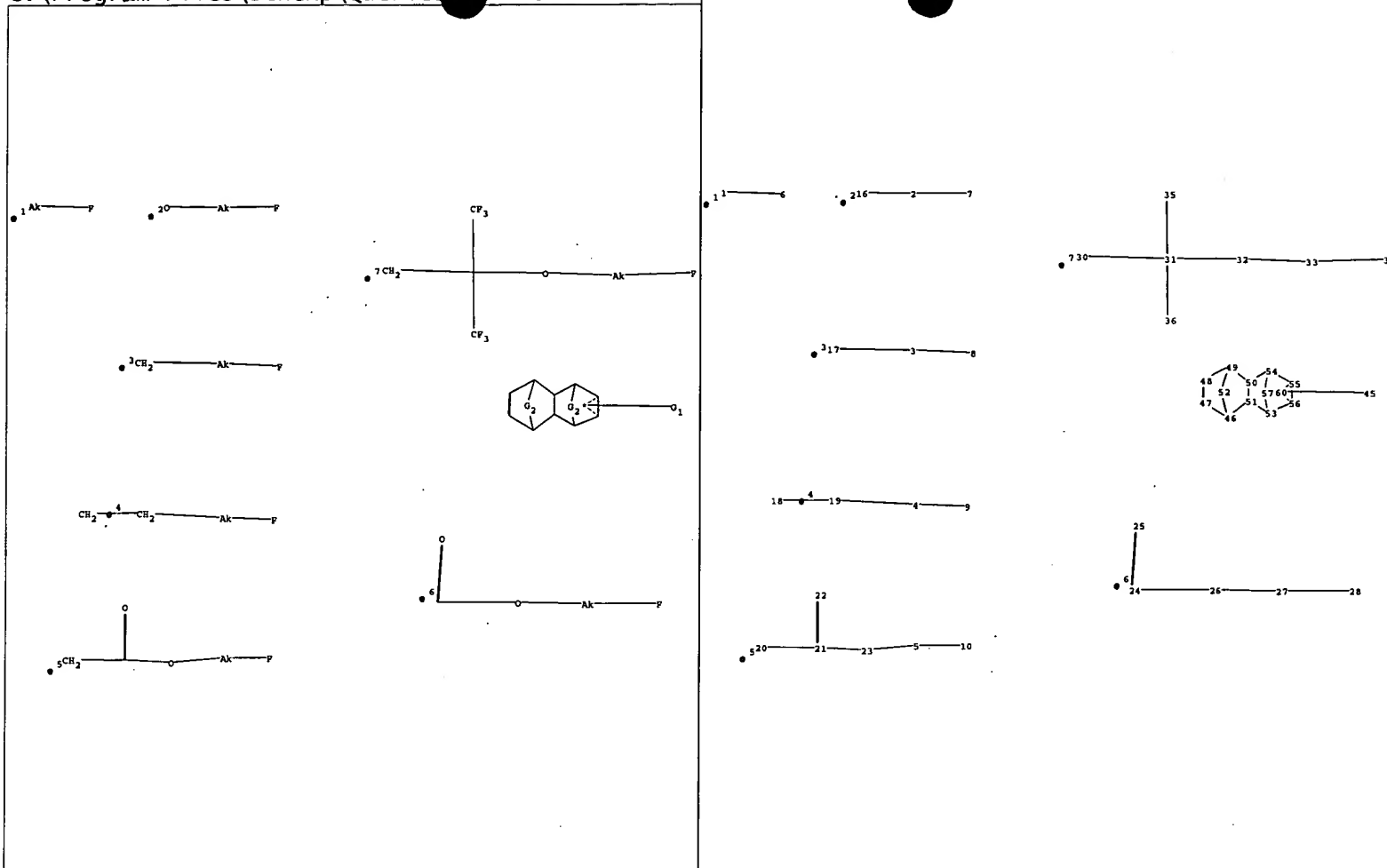
Node 2: Limited
C,C1-6

. Node 3: Limited
C,C1-6

Node 4: Limited
C,C1-6

Node 5: Limited
C,C1-6

Node 27: Limited
C,C1-6



chain nodes :

1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 22 23 24 25 26 27 28 30 31
32 33 34 35 36 45

ring nodes :

46 47 48 49 50 51 52 53 54 55 56 57

chain bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

ring bonds :

46-47 46-51 46-52 47-48 48-49 49-50 49-52 50-54 50-51 51-53 53-57 53-56 54-57
54-55 55-56

exact/norm bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

exact bonds :

46-47 46-51 46-52 47-48 48-49 49-50 49-52 50-54 50-51 51-53 53-57 53-56 54-57
54-55 55-56

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

G2:O,S,NH

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 16:Atom
17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
27:Atom 28:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom
56:Atom 57:Atom 60:CLASS

Element Count :

Node 1: Limited
C,C1-6

Node 2: Limited

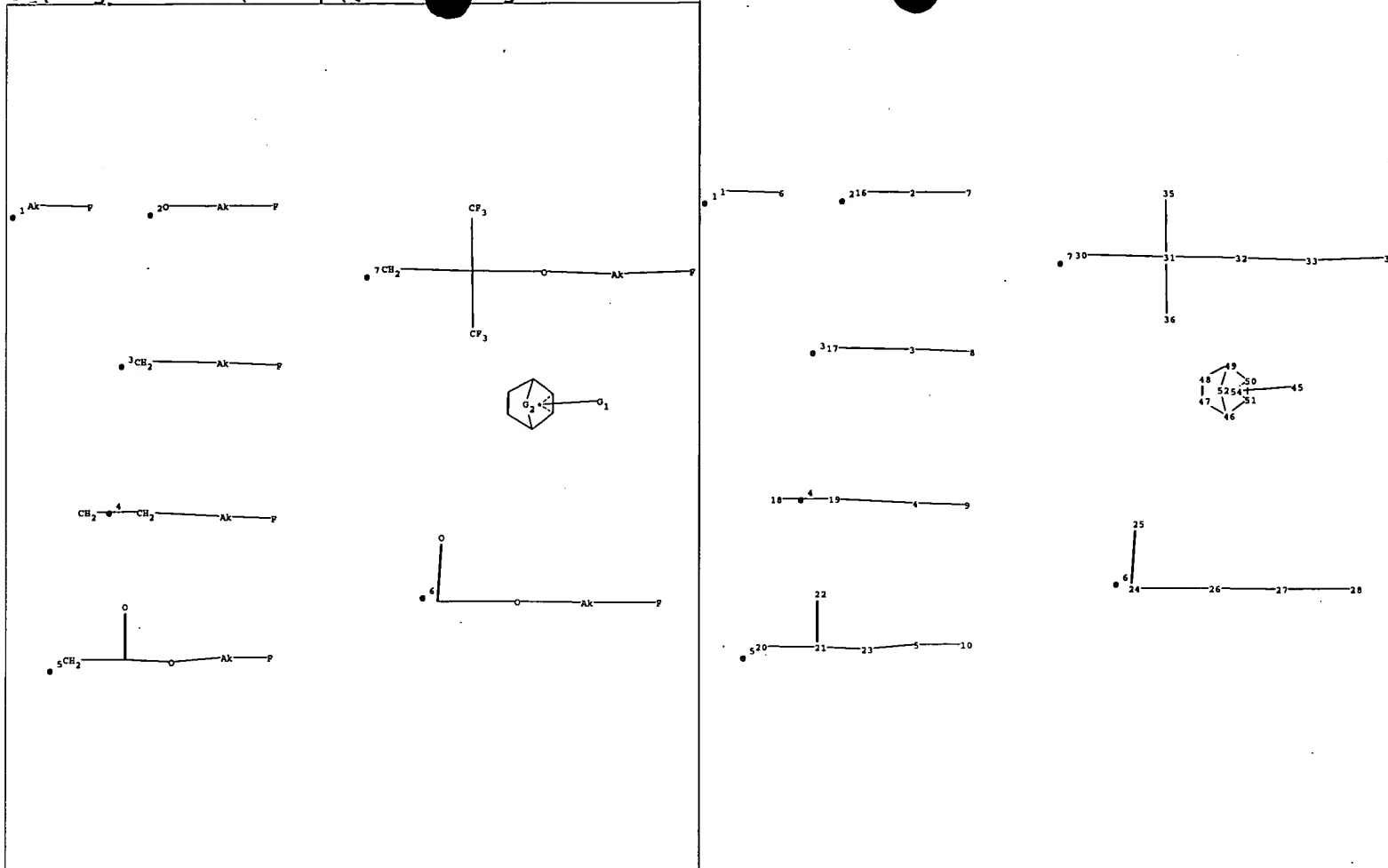
C,C1-6

Node 3: Limited
C,C1-6

Node 4: Limited
C,C1-6

Node 5: Limited
C,C1-6

Node 27: Limited
C,C1-6



chain nodes :

1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 22 23 24 25 26 27 28 30 31
32 33 34 35 36 45

ring nodes :

46 47 48 49 50 51 52

chain bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

ring bonds :

46-47 46-51 46-52 47-48 48-49 49-50 49-52 50-51

exact/norm bonds :

1-6 2-7 2-16 3-8 3-17 4-9 4-19 5-10 5-23 18-19 20-21 21-22 21-23 24-25 24-26
26-27 27-28 30-31 31-32 31-35 31-36 32-33 33-34

exact bonds :

46-47 46-51 46-52 47-48 48-49 49-50 49-52 50-51

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

G2:O,S,NH

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 16:Atom
17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
27:Atom 28:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 45:Atom
46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 54:CLASS

Element Count :

Node 1: Limited
C,C1-6

Node 2: Limited
C,C1-6

Node 3: Limited

- G,C1-6

Node 4: Limited
C,C1-6

Node 5: Limited
C,C1-6

Node 27: Limited
C,C1-6